Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims

1. (currently amended):   A method for selecting at least one lead-candidate compound capable of binding as a ligand to a ~~biopolymer~~ protein from a compound database comprising information on atomic types and covalent bonds of compounds in the database, comprising: ~~selecting at least one trial compound by matching at least one query molecule capable of binding to the biopolymer with trial compounds stored in the database for the mode of covalent bond~~

a) choosing at least one query molecule that is known to bind, or expected to be capable of binding, to the protein; and

b) selecting lead-candidate compounds from the compound database by matching modes of covalent bonds between the query molecule and a trial compound stored in the database and judging similarity of partial structures of the query molecule and the trial compound.

2-5. (canceled)

6. (currently amended)   The method of claim 1, ~~further comprising~~ wherein the compound database comprises information on three-dimensional structures of the

compounds, and which further comprises:

~~estimating binding schemes of the trial compounds to the biopolymer based on~~ ~~the binding schemes of the at least one query molecule to the biopolymer;~~

~~calculating at least one parameter relating to interaction between the trial~~ ~~compounds and the biopolymer; and~~

~~screening the trial compounds based on the parameters~~

c) estimating a binding scheme of the lead-candidate compound selected in step b) to the protein based on three-dimensional information and binding scheme to the protein of the query molecule and based on correspondence of the partial structures of the query molecule and the trail compound;

d) calculating one or more parameters relating to interaction between the lead-candidate compound and the protein; and

e) screening the lead-candidate compounds based on the parameters calculated in step d).

7. (currently amended):   The method of claim 1, ~~further comprising~~ wherein the compound database comprises information on three-dimensional structures of the compounds, and which further comprises:

c) estimating a virtual receptor model which represents physicochemical environment of the ligand binding site of the ~~biopolymer~~ protein based on information of three-dimensional structures of one or more known ligands capable of binding to the ~~biopolymer~~ protein;

d) fitting the lead-candidate compound selected in step b) to the virtual receptor

model and judging goodness of fit of the trial compounds to the virtual receptor model;

and

e) screening the trial compounds based on the goodness of fit.

8-10. (canceled)

11. (new) The method of claim 1, further comprising constructing the structure

of the at least one query molecule by an automatic structure construction method.

12. (new) The method of claim 6, further comprising constructing the structure

of the at least one query molecule by an automatic structure construction method.

13. (new) The method of claim 7, further comprising constructing the structure

of the at least one query molecule by an automatic structure construction method.